17beta-Acetoxy-10-isoandrost-4-en-3-one

Other names:	Methyl 3-keto-4-etiocholenate
	4-Androstene-17-carboxylic acid, 3-oxo-, methyl ester
	Androst-4-ene-17-carboxylic acid, 3-oxo-, methyl ester, (17«beta»)-
	Methyl 3-oxo-4-androstene-17beta-carboxylate
	Methyl-3-oxoandrost-4-ene-17B-carboxylate
Inchi:	InChI=1S/C21H30O3/c1-20-10-8-14(22)12-13(20)4-5-15-16-6-7-18(19(23)24-3)21(16,2)1
InchiKey:	XWFWMYFLNHTEBF-NLPWGACESA-N
Formula:	C21H30O3
SMILES:	COC(=O)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	330.46
CAS:	2681-55-2

Physical Properties

Property code	Value	Unit	Source
gf	-54.14	kJ/mol	Joback Method
hf	-562.76	kJ/mol	Joback Method
hfus	24.86	kJ/mol	Joback Method
hvap	74.29	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.307		Crippen Method
mcvol	268.020	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	2730.00		NIST Webbook
tb	867.58	K	Joback Method
tc	1115.31	K	Joback Method
tf	573.57	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.49	J/mol×K	867.58	Joback Method
cpg	971.99	J/mol×K	908.87	Joback Method
cpg	998.46	J/mol×K	950.16	Joback Method

cpg	1025.25	J/mol×K	991.45	Joback Method
cpg	1052.70	J/mol×K	1032.74	Joback Method
cpg	1081.18	J/mol×K	1074.03	Joback Method
cpg	1111.01	J/mol×K	1115.31	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2681552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume